Applied Mathematics Letters 22 (2009) 147–152

Contents lists available at ScienceDirect

Applied Mathematics Letters

journal homepage: www.elsevier.com/locate/aml

Global-in-time existence of solutions to the multiconfiguration time-dependent Hartree–Fock equations: A sufficient condition

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ARTICLE INFO

Article history:
Received 27 December 2007
Accepted 27 December 2007

Keywords:
MCTDHF system
Linear *N*-particle Schrödinger equation
Few-electron systems
Ground State

ABSTRACT

The multiconfiguration time-dependent Hartree–Fock (MCTDHF for short) system is an approximation of the linear many-particle Schrödinger equation with a binary interaction potential by nonlinear "one-particle" equations. MCTDHF methods are widely used for numerical calculations of the dynamics of few-electron systems in quantum physics and quantum chemistry, but the time-dependent case still poses serious open problems for the analysis, e.g. in the sense that global-in-time existence of solutions is not proved yet. In this letter we present the first result ever where global existence is proved under a condition on the initial datum that it has to be somewhat close to the "ground state".

1. Introduction

The multiconfiguration time-dependent Hartree–Fock (MCTDHF for short) system is an approximation of the linear N-particle Schrödinger equation with a binary interaction potential V. MCTDHF methods are widely used for numerical calculations of the dynamics of few-electron systems in quantum physics and quantum chemistry, but the time-dependent case still poses serious open problems for the analysis in the sense that global-in-time existence of solutions is not proved yet. In this letter we present the first result ever where global existence is proved under a condition on the initial datum that it has to be somewhat close to the "ground state".

The MCTDHF system is composed of $K \geq N$ non-linear Schrödinger-type evolution equations (for "the orbitals", as a dynamic basis for an expansion in "Slater determinants") coupled with $\binom{K}{N}$ ordinary differential equations (for "the coefficients"). The many-particle wavefunction $\Psi^N(x_1, \ldots, x_N, t)$ can be well approximated by such linear combinations of Slater determinants that catch also "correlations", in contrast to the simple time-dependent Hartree–Fock (TDHF) method corresponding to the special case $K = N$. In principle, the many-particle wavefunction constructed from the solution of MCTDHF converges towards the exact solution Ψ^N with increasing K; however, especially in the time-dependent case there is no proof for this seemingly "obvious" property of MCTDHF. For a short and readable introduction to the multiconfiguration time-dependent Hartree–Fock (MCTDHF) system we refer the reader to [10] or, more exhaustive, [6].

The existence and uniqueness of solutions have been established in [9] for bounded and smooth interaction potentials V. The case for the singular Coulomb potential has recently been stated and solved in [10,4]. All these results, however, are

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doi:10.1016/j.aml.2007.12.033

local-in-time ones in the sense that the existence, uniqueness and regularity persist only as long as the first-order density operator associated with the system remains of maximal rank. In the case of a "loss of rank" at a certain time T^*, the well-posedness holds only locally in time until T^*.

In this letter, we show how the global-in-time existence can be assured under an assumption on the energy of the initial state Ψ_I^N that will usually be in the "energy space" $H^1(\Omega)^N$, where Ω is the spatial domain.

We prove our result in two somewhat simplified situations: for the finite "discrete case" (i.e. Ω bounded and equipped with the Dirac measure) and for the case where Ω is a bounded subset of $\mathbb{R}^3$ with binary interactions as singular as the Coulomb potential, but strictly positive. The general case in $\Omega = \mathbb{R}^3$ is more technical and will be considered in a forthcoming publication [1].

Let Ω be a measured domain and $\mathcal{H}$ a bounded (or unbounded) self-adjoint operator acting on $L^2_s(\Omega^N)$, the space of skew-symmetric functions $\Psi^N(x_1, x_2, \ldots, x_N)$ (i.e. for any permutation s of the set $\{1, 2, \ldots, N\}$ with signature $(-1)^s$); one has

$$\Psi(x_{s(1)}, x_{s(2)}, \ldots, x_{s(N)}) = (-1)^s \Psi(x_1, x_2, \ldots, x_N).$$

The purpose of the MCTDHF method is to approximate the evolution of the "exact" solution $\Psi_I^N(x_1, \ldots, x_N, t)$ of the linear N-particle Schrödinger equation

$$i\partial_t \Psi^N = \mathcal{H}\, \Psi^N, \tag{1}$$

with a given initial datum $\Psi_I^N(x_1, \ldots, x_N)$ in $L^2_s(\Omega^N)$.

Take an integer $K \geq N$ (the number K of "orbitals" larger than the number of particles) and take the set $\Sigma_{N,K}$ of strictly increasing maps σ from $\{1, 2 \ldots, N\}$ to $\{1, 2 \ldots, K\}$ ($\#\{\Sigma_{N,K}\} = \binom{K}{N} := r$). The same symbol σ will be used to denote the image of any such map. Then one introduces the set $\mathcal{F}_{N,K}$ of coefficients and orbitals (with $\langle ., . \rangle$ denoting the scalar product in $L^2(\Omega)$) as follows:

$$\mathcal{F}_{N,K}(\Omega) = \left\{ C = (c_\sigma)_{\sigma \in \Sigma_N^K} \in \mathbb{C}^r \,:\, \sum_{\sigma \in \Sigma_{N,K}} |c_\sigma|^2 = 1 \right\} \times \left\{ \Phi = (\phi_1, \ldots, \phi_K) \in L^2(\Omega)^K \,:\, \langle \phi_i,\, \phi_j \rangle = \delta_{i,j} \right\},$$

equipped with the usual norm of $\ell^2(\mathbb{C}^r) \times L^2(\Omega)^K$. With the maps σ and the vector $\Phi = (\phi_1, \phi_2, \ldots, \phi_K)$ one constructs the normalized *Slater determinants*:

$$\Phi_\sigma(t, x_1, \ldots, x_N) = \frac{1}{\sqrt{N!}} \det(\phi_{\sigma(i)}(t, x_j))_{1 \leq i,j \leq N}. \tag{2}$$

The MCTDHF *ansatz* then consists in taking linear combinations of Slater determinants:

$$\pi(C, \Phi) := \Psi = \sum_{\sigma \in \Sigma_N^K} c_\sigma(t)\, \Phi_\sigma(t, x_1, \ldots, x_N). \tag{3}$$

Observe that for any K, K' one has

$$\forall\, K' \leq K \leq \infty \;\Rightarrow\; \pi(\mathcal{F}_{N,K'}) \subseteq \pi(\mathcal{F}_{N,K}) \subseteq L^2_s(\Omega^N). \tag{4}$$

For all N-particle wavefunctions $\Psi \in L^2(\Omega^N)$ we define the corresponding following "one-particle" density matrix via the trace

$$[\Psi \otimes \Psi]_{:1}(t, x, y) = \int_{\Omega^{N-1}} \Psi(t, x, z_2, \ldots, z_N) \overline{\Psi}(t, y, z_2, \ldots, z_N) \mathrm{d}z_2 \ldots \mathrm{d}z_N.$$

Then the "first-order density operator" or "one-particle density operator", which is a self-adjoint non-negative operator on $L^2(\Omega)$, associated with $\pi(C, \phi)$ for $(C, \Phi) \in \mathcal{F}_{N,K}$ is defined *via* its normalized kernel

$$D_1 := N\, [\pi(C, \Phi) \otimes \pi(C, \Phi)]_{:1}(t, x, y) = \sum_{i,j=1}^{K} \gamma_{i,j}(t) \phi_i(t, x) \otimes \overline{\phi}_j(t, y) := [\Gamma \Phi] \otimes \overline{\Phi}, \tag{5}$$

with $\Gamma = (\gamma_{ij})^T$ a positive $K \times K$ Hermitian matrix of trace N. D_1 is then of operator norm less than or equal to 1 (cf. [8], [2, Lemma 5.2]). Moreover $\gamma_{i,j}$ is given by the formula

$$\gamma_{i,j} = \sum_{i \in \sigma, j \in \tau, \sigma \setminus i = \tau \setminus j} (-1)^{\sigma^{-1}(i)} (-1)^{\tau^{-1}(j)} c_\sigma \overline{c_\tau}. \tag{6}$$

Its eigenvalues will be denoted by $0 \leq \gamma_K \leq \gamma_{K-1} \leq \cdots \leq \gamma_1 \leq 1$ and the *"maximal rank hypothesis"* corresponds to the following equivalent statements:

- The rank of the operator D_1 is equal to K.
- The matrix Γ is invertible.
- The smallest eigenvalue γ_K of Γ is strictly positive.

The above construction has been widely used to approximate the "ground state" energy:

$$\mathcal{E}(\mathcal{H}) = \min_{\Psi \in L^2_s(\Omega^N)} \frac{\langle \mathcal{H}\Psi \mid \Psi \rangle}{|\Psi|^2} \tag{7}$$

by

$$\mathcal{E}(K) = \min_{(C,\Phi)\in \mathcal{F}_{N,K}(\Omega)} \mathcal{E}(\pi(C,\Phi)), \quad \text{with } \mathcal{E}(\pi(C,\Phi)) = \langle \mathcal{H}(\pi(C,\Phi)), \pi(C,\Phi)\rangle. \tag{8}$$

Of course we have the following inequality for the energy:

$$\forall K' \le K \le \infty \Rightarrow \mathcal{E}(\mathcal{H}) \le \mathcal{E}(K) \le \mathcal{E}(K'). \tag{9}$$

Finally we recall that in the "physical case", namely in $L^2(\mathbb{R}^{3N})$ with $\mathcal{H}$ being the sum of the "kinetic energy" Laplacian plus the binary interaction V, which is the Coulomb potential,

$$\mathcal{H} = -\sum_{1\le i\le N} \frac{1}{2}\Delta_{x_i} + \sum_{1\le i<j\le N} V(|x_i - x_j|), \tag{10}$$

the above energies are finite and one has always $\mathcal{E}(K) < \mathcal{E}(K-2)$ [6,5].

With the formula (6) one observes that the set $\{(C,\Phi)|(C,\Phi) \subset \mathcal{F}_{N,K}(\Omega)$ such that rank of $(D_1) = K\}$ is open. It will be denoted by $\mathcal{F}^0_{N,K}$.

Finally the MCTDHF dynamic is the flow $\mathcal{S}$ defined on this open subset by the equations

$$\mathrm{i}\frac{\mathrm{d}}{\mathrm{d}t}c_\sigma(t) = \langle \mathcal{H}\Psi \mid \Phi_\sigma\rangle, \tag{11}$$

$$\mathrm{i}\Gamma(t)\frac{\partial}{\partial t}\Phi(t,x) = (I - \mathcal{P}_\Phi)\left[[\nabla_\Phi \Psi]^\star \mathcal{H}\Psi\right], \tag{12}$$

with $\mathcal{P}_\Phi$ denoting the projector onto the space spanned by the ϕ_i's (cf. [3,10,1]).

2. Results and proofs

As it can immediately seen in Eq. (12), the invertibility of the matrix $\Gamma(t)$ is an essential issue for the global existence of solutions to the flow $\mathcal{S}$ and this is the very object of the present letter.

First the diagonalization of the matrix Γ is used:

Lemma 2.1. *For all $0 \le t < T$ let the mapping $t \mapsto (C,\Phi)(t)$ be continuous in $\mathcal{F}^0_{N,K}$ (i.e. with $\Gamma(t)$ of rank K for $0 \le t < T$). Then there exists a unique unitary transformation which effects the mapping $(C,\Phi)(t) \mapsto (C',\Phi')(t)$ and which diagonalizes D_1 (and hence the matrix $\Gamma(t)$). That is,*

$$\pi((C,\Phi)) = \sum_\sigma c_\sigma \Phi_\sigma = \sum_\sigma c'_\sigma \Phi'_\sigma = \pi((C',\Phi')), \qquad D_1 = \sum_{i,j=1}^K \gamma_{i,j}\,\phi_i \otimes \overline{\phi_j} = \sum_{i=1}^K \gamma'_i\,\phi'_i \otimes \overline{\phi'_i}. \tag{13}$$

The crucial non-trivial point in the above statement is the fact that with the full rank hypothesis the unitary transform is uniquely determined.

Now, we claim:

Lemma 2.2. *Let $(C^n,\Phi^n) \in \mathcal{F}^0_{N,K}$ be a sequence that converges weakly towards $(C^\star,\Phi^\star)$ in $\mathbb{C}^r \times L^2(\Omega)^K$.*

Assume that, for fixed $1 \le m \le K$ and $\beta > 0$,

- *The eigenvalues of Γ^n (associated with C^n) satisfy*

$$\begin{cases} \gamma^n_K \le \cdots \le \gamma^n_m \le \cdots \le \gamma^n_1, & \lim_{n\to+\infty} \gamma^n_m = 0, \\ \text{for } 1 \le p \le m-1, & \lim_{n\to+\infty} \gamma^n_p = \gamma^\star_p \ge \beta > 0. \end{cases} \tag{14}$$

- *After diagonalization as in (13), the sequence ${\phi'}^n_i$ satisfies*

$$1 \le p \le m-1 \Rightarrow \lim_{n\to+\infty} \|{\phi'}^n_p - {\phi'}^\star_p\|_{L^2(\Omega)} = 0.$$

Then, the associated sequence of wavefunctions $\Psi^n \in L^2(\Omega^N) = \pi({C'}^n, {\Phi'}^n)$ converge towards

$$\Psi^* := \sum_{\sigma\cap\{m,\ldots,K\}=\emptyset} \left[\lim_{n\to+\infty} c'^n_\sigma\right] \Phi'^*_\sigma.$$

Proof. Using the unitary transformation, we have

$$\Psi^n = \pi((C^n, \Phi^n)) = \pi((C'^n, \Phi'^n)) = \sum_{\sigma\cap\{m,\dots,K\}\neq\emptyset} c'^n_\sigma \Phi'^n_\sigma + \sum_{\sigma\cap\{m,\dots,K\}=\emptyset} c'_\sigma \Phi'^n_\sigma. \tag{15}$$

On one hand, the first sum in (15) converges strongly towards 0 by (14). Indeed,

$$\left\| \sum_{\sigma\cap\{m,\dots,K\}\neq\emptyset} c'^n_\sigma \Phi'^n_\sigma \right\|_{L^2(\Omega^N)} = \sum_{\sigma\cap\{m,\dots,K\}\neq\emptyset} |c'_\sigma|^2 \leq \sum_{m\leq p\leq K} \sum_{p\in\sigma} |c'_\sigma|^2 = \sum_{m\leq p\leq K} \gamma'^n_p \to 0.$$

On the other hand, the second sum in (15) consists of terms of the form

$$c'^n_\sigma \prod_{1,\dots,m\notin\sigma} \phi'^n_{\sigma(k)}\, m.$$

In other words, it is a tensor product of strongly convergent functions in $L^2(\Omega)$. Thus the second sum converges strongly in $L^2(\Omega^N)$ towards $\Psi^\star$. □

Following Lemma 2.2, we have

Corollary 2.3. *With the assumptions of the Lemma 2.2 the wavefunction $\Psi^\star$, which is a priori in $\pi(\mathcal{F}_{N,K})$, is in fact in $\pi(\mathcal{F}_{N,m-1})$.*

To explain our results, first a discrete model is considered, then the extension to the classical "physical" problems in a bounded domain is given.

There are several good reasons for considering a discrete problem. First it may be in itself a model for binary interactions. Second it corresponds to the system which is obtained by any kind of discretization of the continuous problem, in particular when spectral or Galerkin methods are involved. Finally explaining first the discrete model and then the continuous one allows us to clearly see the issues which are related to analysis separately from the ones related to the algebraic structure of the problem.

A "discrete case". This situation corresponds to the case when Ω is a finite set of points of cardinal $\#\Omega = L$. We identify the functions ϕ_k with the vectors $\phi_k(l) \in \mathbb{C}$, $1 \leq l \leq L$. $L^2(\Omega)$ is equipped with the Euclidean scalar product. This provides a natural definition for the projector $\mathcal{P}_\phi$ and the adjoint of $[\nabla_\phi \Psi]$. Next, Let H_0 be a self-adjoint operator in $L^2(\Omega)$ and a potential V represented by a symmetric matrix $(V_{lm})_{1\leq l,m\leq L}$. The discrete Hamiltonian $\mathcal{H}$ is given by the formula

$$(\mathcal{H}u)(l_1 \dots l_N) = \left(\sum_{1\leq i\leq N} H_{0,i} u \right)(l_1 \dots l_N) + \left(\sum_{1\leq i<j\leq N} V_{l_i,l_j} \right) u(l_1 \dots l_N). \tag{16}$$

Then, we have:

Theorem 2.4. *Let the initial data $(C^0, \Phi^0) \in \mathcal{F}_{N,K}$ be such that $\mathcal{E}(\pi(C^0, \Phi^0)) < \mathcal{E}(K-1)$.*

Then the discrete flow $\mathcal{S}$ defined by the discrete version of the system (11) and (12) admits a unique global-in-time solution.

Proof. In this configuration the Eqs. (11) and (12) are purely algebraic. Moreover, the matrix $\Gamma(t=0)$ is of rank K; otherwise the operator D_1 would be of rank less than K and by the "Löwdin theorem" [8] D_1 would then belong to $\pi(\mathcal{F}_{N,K-1})$ which is incompatible with the hypothesis

$$\mathcal{E}(\pi(C^0, \Phi^0)) < \mathcal{E}(K-1). \tag{17}$$

Therefore, the system has a unique local-in-time solution. Moreover, this solution exists as long as $\Gamma(t)$ is invertible. In the sequel, we shall prove by contradiction the non-existence of a time $T^\star$ such that

$$0 \leq t < T^* \Rightarrow \gamma_p(t) > 0 \quad \text{and} \quad \lim_{t<T^*, t\to T^*} \gamma_p(t) = 0 \quad \text{for some } 1 \leq p \leq K.$$

In fact, with the compactness of $\mathcal{F}_{N,K}$, up to extraction of sub-sequences, one can find an integer $1 \leq m \leq K$, a positive real β and a sequence $t_n < T^\star$ and $\lim_{n\to+\infty} t_n = T^\star$ such that

$$\lim_{n\to+\infty} \gamma_m(t_n) = 0, \quad 0 < \beta \leq \gamma_{m-1}(t_n) \quad \text{and} \quad \lim_{n\to+\infty} (C(t_n), \Phi(t_n)) = (C^*, \Phi^*) \in \mathcal{F}_{N,K}.$$

Then, in the situation of the Lemma 2.2, $\phi_p(t_n)$ converges toward $\phi^\star_p$ for all p, in particular for $1 \leq p \leq m-1$. Since the model is discrete, the strong convergence of the $\phi_p(t_n)$ for all $1 \leq p \leq m-1$ is obvious. Hence, from the Corollary 2.3, one deduces that $\Psi^\star = \pi(C^\star, \Phi^\star)$ belongs in fact to $\pi(\mathcal{F}_{N,m-1})$. Now, by the conservation of the energy, the continuity, and (9), one obtains the following contradiction:

$$\mathcal{E}(K-1) > \mathcal{E}(\Psi(t=0)) = \mathcal{E}(\Psi^n) = \mathcal{E}(\Psi^\star) \geq \mathcal{E}(m-1) \geq \mathcal{E}(K-1). \quad \square$$

The continuous "physical case". In the setting of a continuous space variable $x \in \Omega$, we now write the potential as follows:

$$V(|x|) = \frac{a}{|x|} + V_{\text{reg}}(|x|) \quad \text{with } a \geq 0 \quad \text{and} \quad V_{\text{reg}} \in L^\infty, \tag{18}$$

and we take again (10) for the Hamiltonian $\mathcal{H}$ in $L^2_s(\Omega^N)$.

The following local-in-time result holds:

Theorem 2.5. *Let $(C^0, \Phi^0) \in \mathcal{F}^0_{N,K}(\Omega)$ be an initial data such that $\mathcal{E}(\pi(C^0, \Phi^0)) < \infty$. Then, the flow $\mathcal{S}$ defined by (10)–(12) has a unique local-in-time solution for $t \in (-T^*, T^*)$ with $T^* > 0$. In particular, the matrix $\Gamma(t)$ is invertible on this time interval and the system preserves its total energy*

$$\mathcal{E}(\pi(C(t), \Phi(t))) = \mathcal{E}\left(\pi(C^0, \Phi^0)\right). \tag{19}$$

Furthermore, this solution can be uniquely extended as long as this matrix $\Gamma(t)$ remains invertible.

This theorem has already been proven for a bounded and smooth binary interacting potential ($a = 0$ in (18); cf. [9]) and for the Coulomb potential ($0 < a$; cf. [10,4]). In a simplified setting we now take Ω be an open and bounded domain of $\mathbb{R}^3$ with boundary $\partial\Omega$ and impose a homogeneous Dirichlet boundary condition:

$$\Psi = 0 \quad \text{on } \partial(\Omega)^N.$$

Then for a global-in-time result we have now the following:

Theorem 2.6. *Let $\mathcal{H}$ be as in (10) and let the initial data $(C^0, \Phi^0) \in \mathcal{F}_{N,K}$ and $\Phi^0 \in H^1(\Omega)^K$ be such that $\mathcal{E}(\pi(C^0, \Phi^0)) < \mathcal{E}(K-1)$. Then, the flow $\mathcal{S}$ defined by (10)–(12) has a unique global-in-time solution in $\ell^2(\mathbb{C}^r) \times H^1(\Omega)^K$.*

Proof. We can conclude by contradiction (as in the discrete case), using the conservation of energy and the fact that the injection of $H^1(\Omega)$ in $L^2(\Omega)$ is compact—which is precisely the point where the simplification of bounded Ω is used.

If $\Gamma(t)$ becomes degenerate at $T^\star$, then there exist a sequence t_n and an integer $1 \leq m \leq K$ such that

$$\lim_{n\to\infty} \gamma_m(t_n) = 0 \quad \text{and} \quad 0 < \beta \leq \gamma_{m-1}(t_n).$$

Now, in order to adapt the proof done in the discrete case, it is enough to show that:

- $\lim_{n\to+\infty} \mathcal{E}(\pi(C^n, \Phi^n)) \geq \mathcal{E}(\pi(C^*, \Phi^*))$.
- For $1 \leq p \leq m-1$, the sequence $\phi^n_p = \phi_p(t_n)$ stays in a relatively compact set of $L^2(\Omega)$.

The first point is a consequence of the lower semi-continuity of the energy (see [7] and add V_{reg}). We shall use the conservation of the energy in order to prove the second point. In fact, for $0 \leq t_n < T^\star$, we have

$$\begin{aligned}\mathcal{E}(\pi((C^0, \Phi^0))) &= \mathcal{E}(\pi(C^n, \Phi^n)) \\ &= \int_{\Omega^N} \left[\frac{1}{2}|\nabla\Psi(t_n)|^2 + \left(\sum_{1\leq i<j\leq N} V(|x_i - x_j|)\right)|\Psi(t_n)|^2\right] \mathrm{d}x_1, \ldots, \mathrm{d}x_N.\end{aligned}$$

Now, the Coulomb constant a in (18) being positive and $V_{\text{reg}} \in L^\infty$, one deduces the existence of a non-negative constant $b < \infty$ such that

$$b \geq \frac{1}{2}\int_{\Omega^N} |\nabla\Psi(t_n)|^2 \mathrm{d}x_1, \ldots, \mathrm{d}x_N = \frac{1}{2}\int_\Omega (\Gamma(t_n)\nabla\Phi(t_n), \nabla\Phi(t_n))\,\mathrm{d}x.$$

Now, using the diagonalization procedure, on obtains (omitting the $'$)

$$b \geq \frac{1}{2}\sum_{1\leq p\leq K} \gamma_p(t_n)\int_\Omega |\nabla\phi_p(t_n)|^2 \mathrm{d}x \geq \beta \sum_{1\leq p\leq m-1}\int_\Omega |\nabla\phi_p(t_n)|^2 \mathrm{d}x.$$

The compactness of $\phi_p(t_n)$ for $1 \leq p \leq m-1$ comes, with the hypothesis of Ω bounded, from the Rellich Theorem. □

3. Conclusion

We have shown that the global-in-time well-posedness of the MCTDHF system (10)–(12) follows from the sufficient condition on the initial data $(C^0, \Phi^0) \in \mathcal{F}_{N,K}$ that its energy is close to the "ground state" energy (7) in the sense that

$$\mathcal{E}(\pi(C^0, \Phi^0)) < \mathcal{E}(K-1). \tag{20}$$

For the sake of simplicity, the electrons–nuclei interaction has been omitted in (10) and the domain Ω is assumed bounded. The extension of our results to these situations will be described in a forthcoming publication [1]; e.g. the case $\Omega = \mathbb{R}^3$ can be handled with the concentration–compactness method of P.L. Lions.

The hypothesis (20) can be viewed as a stability constraint in the sense of numerical analysis. Given any initial $\Psi_I^N \in L_s^2(\Omega^N)$ for the Schrödinger dynamic (1) and any $\epsilon > 0$. Then, there exists, for K large enough, an element $(C^0, \Phi^0) \in \mathcal{F}_{N,K}^0$ such that

$$\| \Psi_I^N - \pi(C^0, \Phi^0) \|_{L^2(\Omega^N)} \leq \epsilon. \tag{21}$$

However the meaning of our result is that, to ensure global existence, the number of orbitals K in the MCTDHF approximation has to be chosen in such a way that the condition (20) on the initial energy is satisfied.

Acknowledgements

This work was supported by the Austrian Ministry of Science via its grant for the WPI, by the Austrian Science Foundation (FWF) via the Wissenschaftkolleg "Differential equations" (W17) and the START Project (Y-137-TEC), by the WWTF (Viennese Science Fund, project MA-45), as well as by the EU funded Marie Curie project DEASE (contract MEST-CT-2005-021122).

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